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Uploading C:\Program Files\Stnexp\Queries\rkk803.str
chain nodes :
13 14
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
2-13 5-8 11-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
11 - 14
exact bonds :
1-2 1-6 2-3 2-13 3-4 4-5 5-6 5-8
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12
isolated ring systems :
containing 1 : 7 :
Hydrogen count :
1:>= minimum 1 3:>= minimum 1 6:>= minimum 1 7:>= minimum 1 9:>= minimum 1
10:>=
minimum 1 12:>= minimum 1
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS
       STRUCTURE UPLOADED
L1
L1 HAS NO ANSWERS
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L1

STR

Structure attributes must be viewed using STN Express query preparation.

=> s 11 ful

FULL SEARCH INITIATED 19:52:04 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 4492 TO ITERATE

100.0% PROCESSED 4492 ITERATIONS 4 ANSWERS

SEARCH TIME: 00.00.01

L2 4 SEA SSS FUL L1

=> d 1-4

L2 ANSWER 1 OF 4 REGISTRY COPYRIGHT 2008 ACS on STN

RN 916155-03-8 REGISTRY

ED Entered STN: 21 Dec 2006

CN Phenol, 4-(4-bromotetrahydro-5-propyl-2H-pyran-2-yl)- (CA INDEX NAME)

MF C14 H19 Br O2

SR CA

LC STN Files: CA, CAPLUS

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 2 REFERENCES IN FILE CA (1907 TO DATE)
- 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L2 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2008 ACS on STN
- RN 879544-24-8 REGISTRY
- ED Entered STN: 06 Apr 2006
- CN Phenol, 4-(tetrahydro-5-propyl-2H-pyran-2-yl)- (CA INDEX NAME)
- MF C14 H20 O2
- SR CA
- LC STN Files: CA, CAPLUS, CASREACT

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L2 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2008 ACS on STN
- RN 879544-22-6 REGISTRY
- ED Entered STN: 06 Apr 2006
- CN Phenol, 4-[(2R,5R)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)
- FS STEREOSEARCH
- MF C14 H20 O2
- SR CA
- LC STN Files: CA, CAPLUS, CASREACT

Relative stereochemistry.

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L2 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2008 ACS on STN

RN 700863-32-7 REGISTRY

ED Entered STN: 29 Jun 2004

CN Phenol, 4-[(2R,5S)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

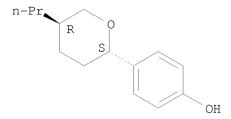
FS STEREOSEARCH

MF C14 H20 O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> fil caplus

SINCE FILE TOTAL ENTRY SESSION 186.36 186.57

COST IN U.S. DOLLARS

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 19:52:14 ON 15 JUL 2008
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FILE COVERS 1907 - 15 Jul 2008 VOL 149 ISS 3 FILE LAST UPDATED: 14 Jul 2008 (20080714/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s 12 L3 6 L2 => d 1-6 bib abs hitstr

L3 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN AN 2006:1252591 CAPLUS <<LOGINID::20080715>>

DN 146:36423

TI Method for producing 2,5-substituted tetrahydropyran derivatives by reductive elimination of the corresponding 4-halogen derivative

IN Poetsch, Eike; Binder, Werner; Lehmann, Stefan; Bensinger, Dieter

PA Merck Patent G.m.b.H., Germany

SO PCT Int. Appl., 72pp. CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 1

	PATENT NO.						D	DATE			APPL					D.	ATE	
ΡI	WO :	 20061	1255	26		A1	_	2006	1130	•			 EP43			2	0060	510
		W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
			CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FΙ,	GB,	GD,
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KM,	KN,	KP,	KR,
			KΖ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,	MW,	MX,
			MZ,	NA,	NG,	NΙ,	NO,	NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,
			SG,	SK,	SL,	SM,	SY,	ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,
			VN,	YU,	ZA,	ZM,	ZW											
		RW:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,
			IS,	ΙΤ,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,
			CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	ΤG,	BW,	GH,
			GM,	KΕ,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,
			KG,	KΖ,	MD,	RU,	ТJ,	TM										
	CN :	10118	3028	7		A		2008	0514	1	CN 2	006-	8001	7968		2	0071	123
	KR :	20080	0190	18		Α		2008	0229		KR 2	007-	7301	62		2	0071	224
PRAI	EP :	2005-	-113	23		Α		2005	0525									
	WO :	2006-	-EP4	387		W		2006	0510									
OS	MAR	PAT 1	146:	3642	3													
GI																		

The invention relates to a method for producing the tetrahydropyran AΒ derivs. I, characterized by subjecting a tetrahydropyran derivative II to a reductive elimination of substituent X1, whereby X1 represents C1, Br, or I. In the general formulas, a, b, c, d, e, and f are independently 0 or 1, and a + b + c + d + e + f equals 0, 1, 2, 3, or 4; R1 is H, halogen, -CN, a C1-C15 alkyl optionally singly substituted with -CN and optionally multiply substituted with -C.tplbond.C-, -CH=CH-, -O-, -S-, -SO-, -SO2-, -CO-O-, or -O-CO-, with no two O atoms adjacent; R2 is independently H, halogen, -CN, -NCS, -NO2, -OH, -SF5, -O-Aralkyl, a C1-C15 alkyl optionally singly substituted with -CN or optionally multiply substituted with halogen, -OH, -O-Aralkyl, -C.tplbond.C-, -CH=CH-, -O-, -S-, -SO-, -SO2-, -CO-O-, or -O-CO-, with no two O atoms adjacent. In the same general formulas, all A groups are 1,4-substituted cyclohexanes or cyclohexenes, 2,5-substituted pyran, 1,3-substituted cyclobutane, a chain of two or three 1,3-connected cyclobutanes, or various ring systems; Z1 is a simple bond, an optionally substituted with F or Cl C1-C6 alkyl bridge, -CH2O-, -OCH2-, or -CF20-; Z2 is a simple bond, or a C1-C6 alkyl bridge optionally substituted with F, Cl, or both; and Z3, Z4, Z5, and Z6 are the same as Z1, except no -CF20- bridge may be connected over its 0-atom directly to a cyclohexylene ring. The tetrahydropyran derivs. function as mesogens in liquid crystal applications and have after synthesis the proper stereochem., in part or in entirety.

IT 700863-32-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (method for producing substituted hydropyran derivs. by reductive elimination of corresponding 4-halogen derivative)

RN 700863-32-7 CAPLUS

CN Phenol, 4-[(2R,5S)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

# RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L3 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2006:1252349 CAPLUS <<LOGINID::20080715>>
- DN 146:36421
- TI Method for producing halogenated tetrahydropyran derivatives for liquid crystal applications
- IN Poetsch, Eike; Binder, Werner; Kirschbaum, Michael; Schaefer, Ralf; Bensinger, Dieter; Nothnagel, Guenther
- PA Merck Patent G.m.b.H., Germany
- SO PCT Int. Appl., 80pp. CODEN: PIXXD2
- DT Patent
- LA German
- FAN.CNT 1

11111.		TENT	NO.			KIN	D	DATE			APPL	ICAT	ION I	NO.		D.	ATE	
ΡI	WO	2006	1255.	 27		A1		2006	1130		WO 2	 006-:	 EP43	 88		2	0060	 510
		W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	AZ,	ΒA,	BB,	BG,	BR,	BW,	BY,	BΖ,	CA,	CH,
			CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KM,	KN,	KP,	KR,
			KΖ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,	MW,	MX,
			MZ,	NA,	NG,	NΙ,	NO,	NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,
			SG,	SK,	SL,	SM,	SY,	ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,
			VN,	YU,	ZA,	ZM,	ZW											
		RW:	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FΙ,	FR,	GB,	GR,	HU,	ΙE,
			IS,	ΙΤ,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,
			CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	ΤG,	BW,	GH,
			GM,	ΚE,	LS,	MW,	MΖ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,
			KG,	KΖ,	MD,	RU,	ТJ,	$_{ m TM}$										
	CN	1011	8028	6		Α		2008	0514	i	CN 2	006-	8001	7926		21	0071	123
	KR	2008	0190	19		Α		2008	0229		KR 2	007-	7301	66		21	0071	224
PRAI	EΡ	2005	-113	25		A		2005	0525									
	WO	2006	-EP4	388		W		2006	0510									
OS	MAF	RPAT	146:	3642	1													

AB The invention relates to a method for producing tetrahydropyran derivs., to the tetrahydropyran derivs., and to the use of the tetrahydropyran derivative for producing other tetrahydropyran derivs. The invention relates

in particular to producing halogenated tetrahydropyran derivs. Synthetic methods are described for producing 2,5-disubstituted tetrahydropyran derivs. that can serve as mesogens in liquid crystal applications. The tetrahydropyran derivs. will already possess the desired stereochem. partly or entirely.

IT 916155-03-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (method for producing halogenated hydropyran derivs. for liquid crystal applications)

RN 916155-03-8 CAPLUS

CN Phenol, 4-(4-bromotetrahydro-5-propyl-2H-pyran-2-yl)- (CA INDEX NAME)

IT 700863-32-7P

RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (method for producing halogenated hydropyran derivs. for liquid crystal applications)

RN 700863-32-7 CAPLUS

CN Phenol, 4-[(2R,5S)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2006:238162 CAPLUS <<LOGINID::20080715>>

DN 144:311909

TI Preparation of trans-2,5-disubstituted tetrahydropyrans

IN Wagner, Robert; Kirschbaum, Michael; Poetsch, Eike; Bensinger, Dieter;
Mueller, Sebastian; Meyer, Volker

PA Merck Patent GmbH, Germany

SO Ger. Offen., 13 pp. CODEN: GWXXBX

DT Patent

LA German

т.	1111 • C111 I				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
Р	I DE 102005032800	A1	20060316	DE 2005-102005032800	20050714
Ρ	RAI DE 2004-10200403751	L4 IA	20040803		
0	S CASREACT 144:311909	)			
G	I				

AB A process for the preparation of title compds. I [X = (Z1-A1)a-R1; Y = (Z2-A2)b-R2; A1, A2 = 1,4-cycloalkylene, 1,4-phenylene, 2,6-naphthyldiyl (sic), etc.; a, b = 0-2; R1, R2 = (un)substituted alkyl with provisos; Z1, Z2 = CH2CH2, (CH2)4, OCF2, etc.] via the isomerization of cis-2,5-disubstituted tetrahydropyrans was disclosed. For example, tribromobismuthine mediated isomerization of a mixture of cis:trans tetrahydropyran II (48:50) in DCM afforded the trans-isomer of tetrahydropyran II in 87%.

IT 879544-22-6

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of trans-2,5-disubstituted tetrahydropyrans)

RN 879544-22-6 CAPLUS

CN Phenol, 4-[(2R,5R)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

IT 879544-24-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of trans-2,5-disubstituted tetrahydropyrans)

RN 879544-24-8 CAPLUS

CN Phenol, 4-(tetrahydro-5-propyl-2H-pyran-2-yl)- (CA INDEX NAME)

IT 700863-32-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of trans-2,5-disubstituted tetrahydropyrans)

RN 700863-32-7 CAPLUS

CN Phenol, 4-[(2R,5S)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

L3 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2004:1035071 CAPLUS <<LOGINID::20080715>>

DN 142:30170

TI Pyrans as liquid crystals for electrooptical and display devices

IN Goulding, Mark John; Duffy, Warren; Adlem, Kevin; Kirsch, Peer; Hahn, Alexander; Poetsch, Eike; Binder, Werner; Meyer, Volker; Klasen-Memmer, Melanie; Heckmeier, Michael; Luessem, Georg

PA Merck Patent GmbH, Germany

SO Eur. Pat. Appl., 22 pp. CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

FAN.	CNT	1																	
	PA:	FENT	NO.			KINI	D	DATE		A)	PPL:	ICAT	ION I	NO.		D.	ATE		
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ΡI	EP	1482	021			A1		2004	1201	El	2 (	004-	1221.	2		2	0040	524	
	ΕP	1482	021			В1		2007	0124										
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			ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY, Z	AL,	TR,	BG,	CZ,	EE,	HU,	PL,	SK,	HR
	ΑT	3526	02			${ m T}$		2007	0215	A'	Г 20	004 - 1	1221.	2		2	0040	524	
	US	2005	0012	073		A1		2005	0120	U	S 20	004-	8547	73		2	0040	527	
	US	7022	865			В2		2006	0404										
PRAI	EΡ	2003	-119	06		A		2003	0527										
OS	MAI	RPAT	142:	3017	0														
GT																			

GΙ

AB Tetrahydropyran derivs. comprising at least three cyclic rings and one aromatic end group of the formula I (X, Y = H, F, with the proviso that at least one of X and Y is F; Q = H, -CN, -NCS, -F, -Cl, -CF3, -OCF3, -OCHF2, -OCHFCF3, SF5 or -OCF2CF3); a process for preparing said tetrahydropyran derivs., and the use of said tetrahydropyran derivs. as a component in a liquid crystal composition. The object of the present invention is to provide

new tetrahydropyran derivs. which are suitable as components in liquid crystalline compns. and display devices, especially in nematic media having a balanced profile of the following properties: rotational viscosity, dielec. anisotropy and holding ratio; and having a good solubility for other components of liquid crystal compns. and a high pos. dielec. anisotropy.

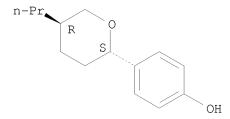
TT 700863-32-7P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent) (preparation of liquid crystals for electrooptical and display devices)

RN 700863-32-7 CAPLUS

CN Phenol, 4-[(2R,5S)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L3 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2004:962862 CAPLUS <<LOGINID::20080715>>
- DN 141:403631
- TI Liquid crystal compound and liquid crystal mixture showing improved physical properties for liquid crystal display
- IN Kirsch, Peer; Hahn, Alexander; Poetsch, Eike; Meyer, Volker; Heckmeier, Michael; Klasen-Memmer, Melanie; Luessem, Georg; Hock, Christian
- PA Merck Patent GmbH, Germany
- SO Ger. Offen., 100 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	<del></del>				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	DE 10318420	A1	20041111	DE 2003-10318420	20030424
PRAI	DE 2003-10318420		20030424		
OS	MARPAT 141:403631				

GΙ

$$R^{1}(A^{1}Z^{1})_{a}$$
  $(Z^{2}A^{2})_{b}$   $CF_{2}O(A^{3}Z^{3})_{c}$   $A^{4}R^{2}$ 

AB The title liquid crystal compound is represented by I (R1, R2 = H, halo, C1-15-alkyl, alkoxy; A1-4 = trans-1,4-cyclohexylene, 1,4-phenylene, etc.; Z1-3 = -COO-, -OCO-, -CF2O-, -OCF2-, etc.; a, b, c = 0-3). There are synthesis examples as well as 11 liquid crystal mixture examples.

IT 700863-32-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

 $\hbox{ (preparation of liquid crystal compound and liquid crystal mixture showing improved }$ 

phys. properties for liquid crystal display)

RN 700863-32-7 CAPLUS

CN Phenol, 4-[(2R,5S)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

- L3 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2004:466725 CAPLUS <<LOGINID::20080715>>
- DN 141:44938
- TI Liquid crystalline compound suitable for liquid crystal mixture of liquid crystal display
- IN Kirsch, Peer; Hahn, Alexander; Poetsch, Eike; Meyer, Volker; Heckmeier, Michael; Klasen-Memmer, Melanie; Luessem, Georg; Hock, Christian
- PA Merck Patent G.m.b.H., Germany

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SO
     Ger. Offen., 154 pp.
     CODEN: GWXXBX
DT
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     German
FAN.CNT 1
     PATENT NO.
                        KIND
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                                            APPLICATION NO.
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                         A1 20040609
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     DE 10353658
                                                                    20031117
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                                            WO 2003-EP12813
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             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
             TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
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             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
             TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD,

      20040618
      AU 2003-302394
      20031117

      20050824
      EP 2003-811758
      20031117

     AU 2003302394
                          A1
     EP 1565540
                          Α1
     EP 1565540
                          В1
                                 20070926
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
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                                           CN 2003-80104414 20031117
     JP 2006508150
                          Τ
                                20060309
                                           JP 2004-554363
                                                                     20031117
                          Τ
                               20071015
     AT 374232
                                            AT 2003-811758
                                                                     20031117
                         A1 20060323
B2 20071106
     US 20060061699
                                            US 2005-536808
                                                                     20050527
     US 7291367
                      A1 20021127
W 20031117
PRAI DE 2002-10255311
     WO 2003-EP12813
     MARPAT 141:44938
OS
GΙ
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$$R^{1}$$
 (A<sup>1</sup>-Z<sup>1</sup>)a (Z<sup>2</sup>-A<sup>2</sup>)b-CF<sub>2</sub>O-(A<sup>3</sup>-Z<sup>3</sup>)c-A<sup>4</sup>-R<sup>2</sup>

AB The title liquid crystalline compound is represented by a general formula I (R1, R2  $\,$ 

= H, halo, C1-15-alkyl, alkoxy; A1-4 = 1,4-trans-cyclohexylene, 1,4-phenylene, etc.; Z1-3 = -C00-, -OC0-, -CF20-, etc.; a, b, c = 0-3; a + b + c  $\leq$ 3). Synthesis examples and 45 mixture examples are given.

IT 700863-32-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of liquid crystalline compound suitable for liquid crystal mixture of liquid

crystal display)

RN 700863-32-7 CAPLUS
CN Phenol, 4-[(2R,5S)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

=>

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NEWS 16 MAR 31 CA/Caplus and CASREACT patent number format for U.S.
                 applications updated
NEWS 17 MAR 31
                LPCI now available as a replacement to LDPCI
NEWS 18
        MAR 31
                EMBASE, EMBAL, and LEMBASE reloaded with enhancements
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        APR 04
                STN AnaVist, Version 1, to be discontinued
NEWS 20 APR 15
                WPIDS, WPINDEX, and WPIX enhanced with new
                 predefined hit display formats
NEWS 21
        APR 28
                EMBASE Controlled Term thesaurus enhanced
NEWS 22
        APR 28
                IMSRESEARCH reloaded with enhancements
NEWS 23 MAY 30
                INPAFAMDB now available on STN for patent family
                 searching
NEWS 24
        MAY 30
                DGENE, PCTGEN, and USGENE enhanced with new homology
                 sequence search option
NEWS 25
        JUN 06
                 EPFULL enhanced with 260,000 English abstracts
NEWS 26
        JUN 06
                KOREAPAT updated with 41,000 documents
NEWS 27
        JUN 13
                USPATFULL and USPAT2 updated with 11-character
                 patent numbers for U.S. applications
NEWS 28
        JUN 19
                CAS REGISTRY includes selected substances from
                 web-based collections
NEWS 29
        JUN 25
                CA/CAplus and USPAT databases updated with IPC
                 reclassification data
NEWS 30
        JUN 30
                AEROSPACE enhanced with more than 1 million U.S.
                 patent records
                EMBASE, EMBAL, and LEMBASE updated with additional
NEWS 31
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                 options to display authors and affiliated
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FULL ESTIMATED COST

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chain nodes :
13 14
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
2-13 5-8 11-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
11-14
exact bonds :
1-2 1-6 2-3 2-13 3-4 4-5 5-6 5-8

normalized bonds:
7-8 7-12 8-9 9-10 10-11 11-12 isolated ring systems:
containing 1: 7:

Hydrogen count :

1:>= minimum 1 3:>= minimum 1 6:>= minimum 1 7:>= minimum 1 9:>= minimum 1

minimum 1 12:>= minimum 1

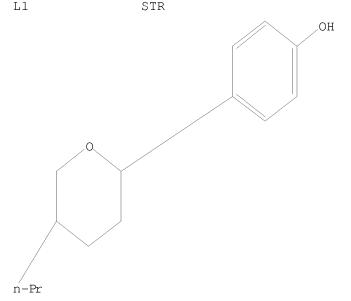
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS

### L1 STRUCTURE UPLOADED

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L1 HAS NO ANSWERS



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FULL SEARCH INITIATED 19:52:04 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 4492 TO ITERATE

100.0% PROCESSED 4492 ITERATIONS 4 ANSWERS SEARCH TIME: 00.00.01

L2 4 SEA SSS FUL L1

=> d 1-4

L2 ANSWER 1 OF 4 REGISTRY COPYRIGHT 2008 ACS on STN

RN 916155-03-8 REGISTRY

ED Entered STN: 21 Dec 2006

CN Phenol, 4-(4-bromotetrahydro-5-propyl-2H-pyran-2-yl)- (CA INDEX NAME)

MF C14 H19 Br O2

SR CA

LC STN Files: CA, CAPLUS

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2008 ACS on STN

RN 879544-24-8 REGISTRY

ED Entered STN: 06 Apr 2006

CN Phenol, 4-(tetrahydro-5-propyl-2H-pyran-2-yl)- (CA INDEX NAME)

MF C14 H20 O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- L2 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2008 ACS on STN
- RN 879544-22-6 REGISTRY
- ED Entered STN: 06 Apr 2006
- CN Phenol, 4-[(2R,5R)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)
- FS STEREOSEARCH
- MF C14 H20 O2
- SR CA

LC STN Files: CA, CAPLUS, CASREACT

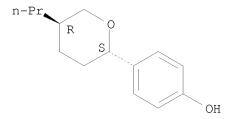
Relative stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- L2 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2008 ACS on STN
- RN 700863-32-7 REGISTRY
- ED Entered STN: 29 Jun 2004
- CN Phenol, 4-[(2R,5S)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)
- FS STEREOSEARCH
- MF C14 H20 O2
- SR CA
- LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

6 REFERENCES IN FILE CA (1907 TO DATE)
6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> fil caplus COST IN U.S. DOLLARS

0001 111 0.0. 20111110

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 186.36 186.57

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=> s 12 L3 6 L2

=> d 1-6 bib abs hitstr

- L3 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2006:1252591 CAPLUS <<LOGINID::20080715>>
- DN 146:36423
- TI Method for producing 2,5-substituted tetrahydropyran derivatives by reductive elimination of the corresponding 4-halogen derivative
- IN Poetsch, Eike; Binder, Werner; Lehmann, Stefan; Bensinger, Dieter
- PA Merck Patent G.m.b.H., Germany
- SO PCT Int. Appl., 72pp.

CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 1

	PATENT 1	KIN	D	DATE			APPL	ICAT	ION I	NO.		D	ATE				
						_									_		
ΡI	WO 2006125526			A1		2006	1130		WO 2	006-	EP43	87		2	0060	510	
	W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KM,	KN,	KP,	KR,
		KΖ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,	MW,	MX,
		ΜZ,	NA,	NG,	NΙ,	NO,	NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,
		SG,	SK,	SL,	SM,	SY,	ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UΖ,	VC,
		VN,	YU,	ZA,	ZM,	ZW											
	RW:	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,
		IS,	ΙΤ,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,

AΒ The invention relates to a method for producing the tetrahydropyran derivs. I, characterized by subjecting a tetrahydropyran derivative II to a reductive elimination of substituent X1, whereby X1 represents C1, Br, or I. In the general formulas, a, b, c, d, e, and f are independently 0 or 1, and a + b + c + d + e + f equals 0, 1, 2, 3, or 4; R1 is H, halogen, -CN, a C1-C15 alkyl optionally singly substituted with -CN and optionally multiply substituted with -C.tplbond.C-, -CH=CH-, -O-, -S-, -SO-, -SO2-, -CO-O-, or -O-CO-, with no two O atoms adjacent; R2 is independently H, halogen, -CN, -NCS, -NO2, -OH, -SF5, -O-Aralkyl, a C1-C15 alkyl optionally singly substituted with -CN or optionally multiply substituted with halogen, -OH, -O-Aralkyl, -C.tplbond.C-, -CH=CH-, -O-, -S-, -SO-, -SO2-, -CO-O-, or -O-CO-, with no two O atoms adjacent. In the same general formulas, all A groups are 1,4-substituted cyclohexanes or cyclohexenes, 2,5-substituted pyran, 1,3-substituted cyclobutane, a chain of two or three 1,3-connected cyclobutanes, or various ring systems; Z1 is a simple bond, an optionally substituted with F or Cl C1-C6 alkyl bridge, -CH2O-, -OCH2-, or -CF20-; Z2 is a simple bond, or a C1-C6 alkyl bridge optionally substituted with F, Cl, or both; and Z3, Z4, Z5, and Z6 are the same as Z1, except no -CF20- bridge may be connected over its 0-atom directly to a cyclohexylene ring. The tetrahydropyran derivs. function as mesogens in liquid crystal applications and have after synthesis the proper stereochem., in part or in entirety.

IT 700863-32-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (method for producing substituted hydropyran derivs. by reductive elimination of corresponding 4-halogen derivative)

RN 700863-32-7 CAPLUS

CN Phenol, 4-[(2R,5S)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX

NAME)

Relative stereochemistry.

IT 916155-03-8

RL: RCT (Reactant); RACT (Reactant or reagent) (method for producing substituted hydropyran derivs. by reductive elimination of corresponding 4-halogen derivative)

RN 916155-03-8 CAPLUS

CN Phenol, 4-(4-bromotetrahydro-5-propyl-2H-pyran-2-yl)- (CA INDEX NAME)

# RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2006:1252349 CAPLUS <<LOGINID::20080715>>

DN 146:36421

- TI Method for producing halogenated tetrahydropyran derivatives for liquid crystal applications
- IN Poetsch, Eike; Binder, Werner; Kirschbaum, Michael; Schaefer, Ralf;
  Bensinger, Dieter; Nothnagel, Guenther

PA Merck Patent G.m.b.H., Germany

SO PCT Int. Appl., 80pp.

CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 1

	PATENT NO.					KIN	D	DATE			APPL	ICAT	I NOI	NO.		D	ATE	
							_											
ΡI	WO	2006	1255	27		A1		2006	1130	,	WO 2	006-	EP43	88		2	0060	510
		W:	ΑE,	ΑG,	AL,	ΑM,	ΑT,	ΑU,	ΑZ,	ΒA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
			CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚM,	KN,	KP,	KR,
			KΖ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,	MW,	MX,
			MZ,	NA,	NG,	NI,	NO,	NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,
			SG,	SK,	SL,	SM,	SY,	TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,

VN, YU, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM CN 101180286 Α 20080514 CN 2006-80017926 20071123 KR 2008019019 20080229 KR 2007-730166 20071224 Α PRAI EP 2005-11325 20050525 Α WO 2006-EP4388 20060510

OS MARPAT 146:36421

AB The invention relates to a method for producing tetrahydropyran derivs., to the tetrahydropyran derivs., and to the use of the tetrahydropyran derivative for producing other tetrahydropyran derivs. The invention relates in particular to producing halogenated tetrahydropyran derivs. Synthetic methods are described for producing 2,5-disubstituted tetrahydropyran derivs. that can serve as mesogens in liquid crystal applications. The tetrahydropyran derivs. will already possess the desired stereochem. partly or entirely.

ΙT 916155-03-8P

> RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (method for producing halogenated hydropyran derivs. for liquid crystal applications)

RN 916155-03-8 CAPLUS

Phenol, 4-(4-bromotetrahydro-5-propyl-2H-pyran-2-yl)- (CA INDEX NAME) CN

ΙT 700863-32-7P

RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (method for producing halogenated hydropyran derivs. for liquid crystal applications)

RN 700863-32-7 CAPLUS

CN Phenol, 4-[(2R,5S)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

## RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L3 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2006:238162 CAPLUS <<LOGINID::20080715>>
- DN 144:311909
- TI Preparation of trans-2,5-disubstituted tetrahydropyrans
- IN Wagner, Robert; Kirschbaum, Michael; Poetsch, Eike; Bensinger, Dieter; Mueller, Sebastian; Meyer, Volker
- PA Merck Patent GmbH, Germany
- SO Ger. Offen., 13 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	DE 102005032800	A1	20060316	DE 2005-102005032800	20050714
PRAI	DE 2004-10200403751	4 IA	20040803		
OS	CASREACT 144:311909				
GI					

- AB A process for the preparation of title compds. I [X = (Z1-A1)a-R1; Y = (Z2-A2)b-R2; A1, A2 = 1,4-cycloalkylene, 1,4-phenylene, 2,6-naphthyldiyl (sic), etc.; a, b = 0-2; R1, R2 = (un)substituted alkyl with provisos; Z1, Z2 = CH2CH2, (CH2)4, OCF2, etc.] via the isomerization of cis-2,5-disubstituted tetrahydropyrans was disclosed. For example, tribromobismuthine mediated isomerization of a mixture of cis:trans tetrahydropyran II (48:50) in DCM afforded the trans-isomer of tetrahydropyran II in 87%.
- IT 879544-22-6
  - RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of trans-2,5-disubstituted tetrahydropyrans)
- RN 879544-22-6 CAPLUS
- CN Phenol, 4-[(2R,5R)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

IT 879544-24-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of trans-2,5-disubstituted tetrahydropyrans)

RN 879544-24-8 CAPLUS

CN Phenol, 4-(tetrahydro-5-propyl-2H-pyran-2-yl)- (CA INDEX NAME)

IT 700863-32-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of trans-2,5-disubstituted tetrahydropyrans)

RN 700863-32-7 CAPLUS

CN Phenol, 4-[(2R,5S)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

- L3 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2004:1035071 CAPLUS <<LOGINID::20080715>>
- DN 142:30170
- TI Pyrans as liquid crystals for electrooptical and display devices
- IN Goulding, Mark John; Duffy, Warren; Adlem, Kevin; Kirsch, Peer; Hahn, Alexander; Poetsch, Eike; Binder, Werner; Meyer, Volker; Klasen-Memmer, Melanie; Heckmeier, Michael; Luessem, Georg
- PA Merck Patent GmbH, Germany
- SO Eur. Pat. Appl., 22 pp.

CODEN: EPXXDW

Patent DTLA English

FAN.CNT 1

T. TATA • (	OTA T																		
	PA:	ΓΕΝΤ	NO.			KINI	)	DATE		AP	PL:	ICAT	ION :	NO.		D.	ATE		
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ΡI	ΕP	1482	021			A1		2004	1201	EP	20	004-	1221	2		2	0040	524	
	ΕP	1482	021			В1		2007	0124										
		R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB, G	R,	ΙT,	LI,	LU,	NL,	SE,	MC,	PT,	
			ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY, A	L,	TR,	BG,	CZ,	EE,	HU,	PL,	SK,	HR
	ΑT	3526	02			${ m T}$		2007	0215	AT	2(	004-	1221	2		2	0040	524	
	US	2005	0012	073		A1		2005	0120	US	20	004-	8547	73		2	0040	527	
	US	7022	865			В2		2006	0404										
PRAI	EP	2003	-119	06		A		2003	0527										
OS	MAI	RPAT	142:	3017	0														
GT																			

AΒ Tetrahydropyran derivs. comprising at least three cyclic rings and one aromatic end group of the formula I (X, Y = H, F, with the proviso that at least one of X and Y is F; Q = H, -CN, -NCS, -F, -C1, -CF3, -OCF3, -OCHF2, -OCHFCF3, SF5 or -OCF2CF3); a process for preparing said tetrahydropyran derivs., and the use of said tetrahydropyran derivs. as a component in a liquid crystal composition The object of the present invention is to provide

tetrahydropyran derivs. which are suitable as components in liquid crystalline compns. and display devices, especially in nematic media having a balanced profile of the following properties: rotational viscosity, dielec. anisotropy and holding ratio; and having a good solubility for other components of liquid crystal compns. and a high pos. dielec. anisotropy.

ΙT 700863-32-7P

new

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of liquid crystals for electrooptical and display devices) 700863-32-7 CAPLUS

RN

Phenol, 4-[(2R,5S)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX CN NAME)

# RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2004:962862 CAPLUS <<LOGINID::20080715>>

DN 141:403631

TI Liquid crystal compound and liquid crystal mixture showing improved physical properties for liquid crystal display

IN Kirsch, Peer; Hahn, Alexander; Poetsch, Eike; Meyer, Volker; Heckmeier, Michael; Klasen-Memmer, Melanie; Luessem, Georg; Hock, Christian

PA Merck Patent GmbH, Germany

SO Ger. Offen., 100 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	9				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI PRAI OS GI	DE 10318420 DE 2003-10318420 MARPAT 141:403631	A1	20041111 20030424	DE 2003-10318420	20030424

$$R^{1}(A^{1}Z^{1})_{a}$$
  $(Z^{2}A^{2})_{b}$   $CF_{2}O(A^{3}Z^{3})_{c}$   $A^{4}R^{2}$ 

- AB The title liquid crystal compound is represented by I (R1, R2 = H, halo, C1-15-alkyl, alkoxy; A1-4 = trans-1,4-cyclohexylene, 1,4-phenylene, etc.; Z1-3 = -COO-, -OCO-, -CF2O-, -OCF2-, etc.; a, b, c = 0-3). There are synthesis examples as well as 11 liquid crystal mixture examples.
- IT 700863-32-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

 $\hbox{ (preparation of liquid crystal compound and liquid crystal mixture showing improved} \\$ 

phys. properties for liquid crystal display)

RN 700863-32-7 CAPLUS

CN Phenol, 4-[(2R,5S)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

### Relative stereochemistry.

```
L3 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
```

AN 2004:466725 CAPLUS <<LOGINID::20080715>>

DN 141:44938

- TI Liquid crystalline compound suitable for liquid crystal mixture of liquid crystal display
- IN Kirsch, Peer; Hahn, Alexander; Poetsch, Eike; Meyer, Volker; Heckmeier, Michael; Klasen-Memmer, Melanie; Luessem, Georg; Hock, Christian
- PA Merck Patent G.m.b.H., Germany
- SO Ger. Offen., 154 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

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7NHRMN ZEKD77 I 7777

$$R^{1-(A^{1}-Z^{1})a}$$
  $(Z^{2-A^{2}})b-CF_{2}O-(A^{3}-Z^{3})c-A^{4}-R^{2}$ 

AB The title liquid crystalline compound is represented by a general formula I (R1, R2  $\,$ 

= H, halo, C1-15-alkyl, alkoxy; A1-4 = 1,4-trans-cyclohexylene,

1,4-phenylene, etc.; Z1-3 = -C00-, -0C0-, -CF20-, etc.; a, b, c = 0-3; a + b + c  $\leq$ 3). Synthesis examples and 45 mixture examples are given.

IT 700863-32-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

 $\hbox{ (preparation of liquid crystalline compound suitable for liquid crystal } \\ \text{mixture of liquid}$ 

crystal display)

RN 700863-32-7 CAPLUS

CN Phenol, 4-[(2R,5S)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

=> fil reg COST IN U.S. DOLLARS SINCE FILE TOTAL SESSION ENTRY FULL ESTIMATED COST 34.14 220.71 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -4.80-4.80

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http://www.cas.org/support/stngen/stndoc/properties.html

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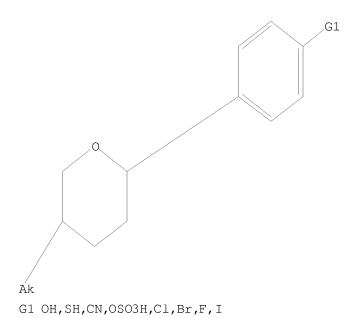
Uploading C:\Program Files\Stnexp\Queries\rkk803b.str

chain nodes :
13 14
ring nodes :

```
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
2-13 5-8 11-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
2-13 11-14
exact bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-8
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12
isolated ring systems :
containing 1 : 7 :
G1:OH, SH, CN, OSO3H, Cl, Br, F, I
Hydrogen count :
1:>= minimum 1 3:>= minimum 1 6:>= minimum 1 7:>= minimum 1 9:>= minimum 1
10:>=
minimum 1 12:>= minimum 1
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS
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### L4 STRUCTURE UPLOADED

=> d L4 HAS NO ANSWERS L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 14 ful

FULL SEARCH INITIATED 19:57:41 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 57439 TO ITERATE

100.0% PROCESSED 57439 ITERATIONS

34 ANSWERS

SEARCH TIME: 00.00.01

L5 34 SEA SSS FUL L4

=> fil caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 180.66 401.37 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL SESSION ENTRY CA SUBSCRIBER PRICE 0.00 -4.80

FILE 'CAPLUS' ENTERED AT 19:57:47 ON 15 JUL 2008
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FILE COVERS 1907 - 15 Jul 2008 VOL 149 ISS 3 FILE LAST UPDATED: 14 Jul 2008 (20080714/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s 15

L6 22 L5

=> d 1-22 bib abs hitstr

L6 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2008:354188 CAPLUS <<LOGINID::20080715>>

DN 148:538015

TI Platinum(II)-catalyzed annulation of 5-methyl-5-hexen-1-ols with aldehydes

AU Miura, Katsukiyo; Horiike, Makoto; Inoue, Gen; Ichikawa, Junji; Hosomi, Akira

CS Department of Chemistry, Graduate School of Pure and Applied Sciences, University of Tsukuba, Tsukuba, 305-8571, Japan

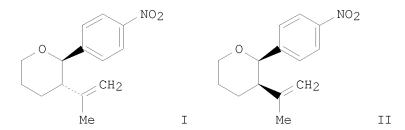
SO Chemistry Letters (2008), 37(3), 270-271 CODEN: CMLTAG; ISSN: 0366-7022

PB Chemical Society of Japan

DT Journal

LA English

GΙ



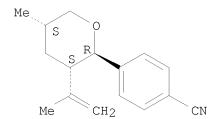
AB In the presence of catalytic amts. of PtC12 and AgOTf, 5-methyl-5-hexen-1-ol reacted with aldehydes to give 2,3-disubstituted tetrahydropyrans in moderate to high yields with trans stereoselectivity. E.g., in the presence of PtC12 and AgOTf, reaction of 5-methyl-5-hexen-1-ol and 4-nitrobenzaldehyde gave 77% trans-tetrahydropyran I and 7% cis-tetrahydropyran II. Use of 5-methyl-5-hexen-1-ols bearing a Me group at the C1-, C2-, or C3-position led to highly stereoselective synthesis of trisubstituted tetrahydropyrans.

IT 1023711-89-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (stereoselective preparation of tetrahydropyrans by PtCl2/AgOTf-catalyzed annulation of 5-methyl-5-hexen-1-ols with aldehydes)

RN 1023711-89-8 CAPLUS

CN Benzonitrile, 4-[(2R,3S,5S)-tetrahydro-5-methyl-3-(1-methylethenyl)-2H-pyran-2-yl]-, rel- (CA INDEX NAME)



## RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2007:85819 CAPLUS <<LOGINID::20080715>>

DN 146:184355

TI Procedure for the production of tetrahydropyrans from 3-oxetanes and imino enolates using Lewis acid mediated addition reaction

IN Kirsch, Peer; Maillard, David

PA Merck Patent GmbH, Germany

SO Ger. Offen., 13pp. CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	DE 102006028618	A1	20070125	DE 2006-102006028618	20060622
PRAI	DE 2005-10200503310	6 IA	20050715		

AB The invention concerns a procedure for the production of 2,5-disubstituted tetrahydropyrans, on the basis of 3-substituted oxetanes and imino enolates. 3-Substituted oxetanes underwent addition of imino enolates under Lewis acid mediated condition to give 2,5-disubstituted tetrahydropyran-2-ols. The 2,5-disubstituted tetrahydropyran-2-ols underwent reductive dehydroxylation to give desired 2,5-disubstituted tetrahydropyrans as the trans-stereoisomers.

IT 911142-61-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of tetrahydropyrans via Lewis acid-mediated addition of imino enolates to oxetanes)

RN 911142-61-5 CAPLUS

CN 2H-Pyran-2-ol, 2-(4-bromophenyl)tetrahydro-5-propyl- (CA INDEX NAME)

IT 700863-30-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of tetrahydropyrans via Lewis acid-mediated addition of imino enolates to oxetanes)

RN 700863-30-5 CAPLUS

CN 2H-Pyran, 2-(4-bromophenyl)tetrahydro-5-propyl-, (2R,5S)-rel- (CA INDEX NAME)

```
ANSWER 3 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
L6
     2006:1252591 CAPLUS <<LOGINID::20080715>>
ΑN
     146:36423
DN
    Method for producing 2,5-substituted tetrahydropyran derivatives by
ΤI
     reductive elimination of the corresponding 4-halogen derivative
     Poetsch, Eike; Binder, Werner; Lehmann, Stefan; Bensinger, Dieter
ΙN
PA
    Merck Patent G.m.b.H., Germany
SO
     PCT Int. Appl., 72pp.
     CODEN: PIXXD2
DT
     Patent
    German
LA
FAN.CNT 1
                        KIND
     PATENT NO.
                                DATE
                                          APPLICATION NO.
                                                                  DATE
                               20061130
                                           WO 2006-EP4387
PΙ
    WO 2006125526
                         A1
                                                                   20060510
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR,
            KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
            MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
             SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
             VN, YU, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
     CN 101180287
                         Α
                                20080514
                                            CN 2006-80017968
                                                                   20071123
     KR 2008019018
                         Α
                                20080229
                                            KR 2007-730162
                                                                   20071224
PRAI EP 2005-11323
                         Α
                                20050525
     WO 2006-EP4387
                                20060510
                         W
    MARPAT 146:36423
OS
GΙ
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The invention relates to a method for producing the tetrahydropyran AΒ derivs. I, characterized by subjecting a tetrahydropyran derivative II to a reductive elimination of substituent X1, whereby X1 represents C1, Br, or I. In the general formulas, a, b, c, d, e, and f are independently 0 or 1, and a + b + c + d + e + f equals 0, 1, 2, 3, or 4; R1 is H, halogen, -CN, a C1-C15 alkyl optionally singly substituted with -CN and optionally multiply substituted with -C.tplbond.C-, -CH=CH-, -O-, -S-, -SO-, -SO2-, -CO-O-, or -O-CO-, with no two O atoms adjacent; R2 is independently H, halogen, -CN, -NCS, -NO2, -OH, -SF5, -O-Aralkyl, a C1-C15 alkyl optionally singly substituted with -CN or optionally multiply substituted with halogen, -OH, -O-Aralkyl, -C.tplbond.C-, -CH=CH-, -O-, -S-, -SO-, -SO2-, -CO-O-, or -O-CO-, with no two O atoms adjacent. In the same general formulas, all A groups are 1,4-substituted cyclohexanes or cyclohexenes, 2,5-substituted pyran, 1,3-substituted cyclobutane, a chain of two or three 1,3-connected cyclobutanes, or various ring systems; Z1 is a simple bond, an optionally substituted with F or Cl C1-C6 alkyl bridge, -CH2O-, -OCH2-, or -CF20-; Z2 is a simple bond, or a C1-C6 alkyl bridge optionally substituted with F, Cl, or both; and Z3, Z4, Z5, and Z6 are the same as Z1, except no -CF20- bridge may be connected over its 0-atom directly to a cyclohexylene ring. The tetrahydropyran derivs. function as mesogens in liquid crystal applications and have after synthesis the proper stereochem., in part or in entirety.

TT 700863-32-7P 916155-28-7P 916155-30-1P 916155-31-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (method for producing substituted hydropyran derivs. by reductive elimination of corresponding 4-halogen derivative)

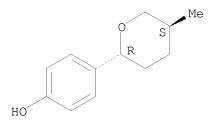
RN 700863-32-7 CAPLUS

CN Phenol, 4-[(2R,5S)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

RN 916155-28-7 CAPLUS

CN Phenol, 4-[(2R,5S)-tetrahydro-5-methyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

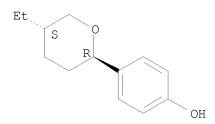
Relative stereochemistry.



RN 916155-30-1 CAPLUS

CN Phenol, 4-[(2R,5S)-5-ethyltetrahydro-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

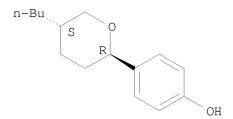
Relative stereochemistry.



RN 916155-31-2 CAPLUS

CN Phenol, 4-[(2R,5S)-5-butyltetrahydro-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



IT 916155-02-7 916155-03-8 916155-04-9

916155-21-0 916155-27-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(method for producing substituted hydropyran derivs. by reductive

elimination of corresponding 4-halogen derivative)

RN 916155-02-7 CAPLUS

CN Phenol, 4-(4-bromo-5-ethyltetrahydro-2H-pyran-2-yl)- (CA INDEX NAME)

RN 916155-03-8 CAPLUS

CN Phenol, 4-(4-bromotetrahydro-5-propyl-2H-pyran-2-yl)- (CA INDEX NAME)

RN 916155-04-9 CAPLUS

CN Phenol, 4-(4-bromo-5-butyltetrahydro-2H-pyran-2-yl)- (CA INDEX NAME)

RN 916155-21-0 CAPLUS

CN 2H-Pyran, 4-bromo-2-(4-bromophenyl)tetrahydro-5-methyl- (CA INDEX NAME)

RN 916155-27-6 CAPLUS

CN Phenol, 4-(4-bromotetrahydro-5-methyl-2H-pyran-2-yl)- (CA INDEX NAME)

IT 916235-98-8P

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(method for producing substituted hydropyran derivs. by reductive elimination of corresponding 4-halogen derivative)

RN 916235-98-8 CAPLUS

CN 2H-Pyran, 2-(4-bromophenyl)tetrahydro-5-methyl-, (2R,5S)-rel- (CA INDEX NAME)

Relative stereochemistry.

# RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L6 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2006:1252349 CAPLUS <<LOGINID::20080715>>
- DN 146:36421
- TI Method for producing halogenated tetrahydropyran derivatives for liquid crystal applications
- IN Poetsch, Eike; Binder, Werner; Kirschbaum, Michael; Schaefer, Ralf; Bensinger, Dieter; Nothnagel, Guenther
- PA Merck Patent G.m.b.H., Germany
- SO PCT Int. Appl., 80pp.

CODEN: PIXXD2

- DT Patent
- LA German
- FAN.CNT 1

		PATENT NO.						KIND DATE		APPLICATION NO.						DATE				
PΙ		WO 2006125527				A1 20061130		WO 2006-EP4388						20060510						
			W:	ΑE,	AG,	AL,	ΑM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,	
				CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
				GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚM,	KN,	KP,	KR,	
				KΖ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	
				MΖ,	NA,	NG,	NI,	NO,	NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	
				SG,	SK,	SL,	SM,	SY,	ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	
				VN,	YU,	ZA,	ZM,	ZW												

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM 20080514 CN 2006-80017926 CN 101180286 Α 20071123 KR 2008019019 Α 20080229 KR 2007-730166 20071224 PRAI EP 2005-11325 Α 20050525 WO 2006-EP4388 W 20060510 OS MARPAT 146:36421

AB The invention relates to a method for producing tetrahydropyran derivs., to the tetrahydropyran derivs., and to the use of the tetrahydropyran derivative for producing other tetrahydropyran derivs. The invention relates in particular to producing halogenated tetrahydropyran derivs. Synthetic methods are described for producing 2,5-disubstituted tetrahydropyran derivs. that can serve as mesogens in liquid crystal applications. The tetrahydropyran derivs. will already possess the desired stereochem. partly or entirely.

IT 916155-02-7P 916155-03-8P 916155-04-9P 916155-21-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (method for producing halogenated hydropyran derivs. for liquid crystal applications)

RN 916155-02-7 CAPLUS

CN Phenol, 4-(4-bromo-5-ethyltetrahydro-2H-pyran-2-yl)- (CA INDEX NAME)

RN 916155-03-8 CAPLUS

CN Phenol, 4-(4-bromotetrahydro-5-propyl-2H-pyran-2-yl)- (CA INDEX NAME)

RN 916155-04-9 CAPLUS CN Phenol, 4-(4-bromo-5-butyltetrahydro-2H-pyran-2-yl)- (CA INDEX NAME)

RN 916155-21-0 CAPLUS

CN 2H-Pyran, 4-bromo-2-(4-bromophenyl)tetrahydro-5-methyl- (CA INDEX NAME)

IT 700863-32-7P 916155-28-7P 916155-30-1P

916155-31-2P

RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (method for producing halogenated hydropyran derivs. for liquid crystal

applications)
RN 700863-32-7 CAPLUS

CN Phenol, 4-[(2R,5S)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

RN 916155-28-7 CAPLUS

CN Phenol, 4-[(2R,5S)-tetrahydro-5-methyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

RN 916155-30-1 CAPLUS

CN Phenol, 4-[(2R,5S)-5-ethyltetrahydro-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

RN 916155-31-2 CAPLUS

CN Phenol, 4-[(2R,5S)-5-butyltetrahydro-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

IT 916155-27-6

RL: RCT (Reactant); RACT (Reactant or reagent) (method for producing halogenated hydropyran derivs. for liquid crystal applications)

RN 916155-27-6 CAPLUS

CN Phenol, 4-(4-bromotetrahydro-5-methyl-2H-pyran-2-yl)- (CA INDEX NAME)

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2006:1250462 CAPLUS <<LOGINID::20080715>>

DN 146:16407

TI Liquid crystalline medium and electrooptical liquid crystal display

IN Wittek, Michael; Lietzau, Lars; Poetsch, Eike; Czanta, Markus

PA Merck Patent G.m.b.H., Germany

SO Ger. Offen., 48pp.

CODEN: GWXXBX

DT Patent

LA German FAN.CNT 1

T 2 21							
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
ΡI	DE 102006020181	A1	20061130	DE 2006-102006020181	20060502		
	DE 102006023335	A1	20061130	DE 2006-102006023335	20060518		
	JP 2006328400	A	20061207	JP 2006-144876	20060525		
PRA	I DE 2005-10200502461	.3 IA	20050525				
OS	MARPAT 146:16407						

GΙ

Ι

 ${\tt AB}$  The present invention relates to nematic liquid crystalline media containing one or

more compds. represented by I (R1 = H, C1-7-alkyl, alkoxy, C2-7-alkenyl, alkenyloxy, alkynyl, alkynyloxy; Z1 = -CH2CH2-, -CH2O-, -CF2O-, -COO-, -OCO-, single bond; X1 = halo, C1-5-fluoroalkyl, fluoroalkoxy, C2-4-fluoroalkenyl, alkenyloxy, oxaalkyl; Y11, Y12 = H, F) and to electrooptical (TN-, OCB-, or IPS-) liquid crystal displays using the same. 915716-78-8 915716-79-9

RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(liquid crystal mixture; nematic liquid crystalline medium and electrooptical liquid  $\ensuremath{\mathsf{e}}$ 

crystal display)

RN 915716-78-8 CAPLUS

CN 2H-Pyran, 2-(4-chlorophenyl)tetrahydro-5-propyl-, (2R,5S)-rel- (CA INDEX NAME)

Relative stereochemistry.

RN 915716-79-9 CAPLUS

CN 2H-Pyran, 5-butyl-2-(4-chlorophenyl)tetrahydro-, (2R,5S)-rel- (CA INDEX NAME)

Relative stereochemistry.

- L6 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2006:1118154 CAPLUS <<LOGINID::20080715>>
- DN 145:443780
- TI Nitric oxide (NO) formation inhibitory compounds, their manufacture by extraction from Alpinia galanga, and antiallergy agents containing them
- IN Yoshikawa, Masayuki; Matsuda, Hisashi; Muraoka, Osamu
- PA Kinki University, Japan; Diabetym Co., Ltd.
- SO Jpn. Kokai Tokkyo Koho, 12pp. CODEN: JKXXAF
- DT Patent
- LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
ΡI	JP 2006290847	A	20061026	JP 2005-117581	20050414		
PRAI	JP 2005-117581		20050414				

AB Galanganal (I), galanganol A (II), galanganol B (III), and galanganol C (IV) are manufactured by chromatog. fractionation of exts. obtained by extraction of

rhizome of Alpinia galanga with an aqueous solution containing  $\geq \! 15$  weight% Me2CO

or lower alcs. I, II (enantiomeric mixture), III (enantiomeric mixture), and IV (enantiomeric mixture) were purified from 80% aqueous Me2CO extract of

of A. galanga, and their structures were elucidated. I, III, and IV inhibited NO formation in cultured mouse cells with IC50 of 68, 88, and 33  $\mu\text{M},$  resp.

IT 864073-18-7P, Galanganol C

RL: NPO (Natural product occurrence); PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)

(extraction of nitric oxide (NO) formation inhibitory galanganal and galanganols A-C from rhizome of Alpinia galanga for antiallergy agents)

RN 864073-18-7 CAPLUS

CN 2H-Pyran-3-methanol, tetrahydro- $\alpha$ ,6-bis(4-hydroxyphenyl)-5-[(2E)-3-(4-hydroxyphenyl)-2-propen-1-yl]-, (3R,5R,6R)-rel- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.
Currently available stereo shown.

- L6 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2006:809645 CAPLUS <<LOGINID::20080715>>
- DN 145:408019
- TI A convenient synthetic route to tetrahydropyran-based liquid crystals
- AU Kirsch, Peer; Maillard, David
- CS Technical Center Atsugi, Merck Ltd. Japan, 4084 Nakatsu, Aikawa-machi, Aiko-gun, Kanagawa, 243-0303, Japan
- SO European Journal of Organic Chemistry (2006), (15), 3326-3331 CODEN: EJOCFK; ISSN: 1434-193X
- PB Wiley-VCH Verlag GmbH & Co. KGaA
- DT Journal
- LA English
- OS CASREACT 145:408019
- AB The tetrahydropyran moiety was identified as a highly advantageous addition to the toolbox for the design of nematic liquid crystals for LCD applications. A new synthetic procedure based on the Lewis acid catalyzed ring opening of oxetanes by Li iminoenolates followed by reductive dehydroxylation of the resulting hemiketal provides a convenient preparative access to this class of materials.
- IT 911142-61-5P
  - RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
    - (preparation and reaction with cyclohexylimine derivs.)
- RN 911142-61-5 CAPLUS
- CN 2H-Pyran-2-ol, 2-(4-bromophenyl)tetrahydro-5-propyl- (CA INDEX NAME)

IT 700863-30-5P

RN 700863-30-5 CAPLUS

CN 2H-Pyran, 2-(4-bromophenyl)tetrahydro-5-propyl-, (2R,5S)-rel- (CA INDEX NAME)

Relative stereochemistry.

RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2006:238162 CAPLUS <<LOGINID::20080715>>

DN 144:311909

TI Preparation of trans-2,5-disubstituted tetrahydropyrans

IN Wagner, Robert; Kirschbaum, Michael; Poetsch, Eike; Bensinger, Dieter;
Mueller, Sebastian; Meyer, Volker

PA Merck Patent GmbH, Germany

SO Ger. Offen., 13 pp. CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	9				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	DE 102005032800	A1	20060316	DE 2005-102005032800	20050714
PRAI	DE 2004-10200403751	4 IA	20040803		
OS	CASREACT 144:311909				
GI					

AB A process for the preparation of title compds. I [X = (Z1-A1)a-R1; Y = (Z2-A2)b-R2; A1, A2 = 1,4-cycloalkylene, 1,4-phenylene, 2,6-naphthyldiyl (sic), etc.; a, b = 0-2; R1, R2 = (un)substituted alkyl with provisos; Z1,

Z2 = CH2CH2, (CH2)4, OCF2, etc.] via the isomerization of cis-2,5-disubstituted tetrahydropyrans was disclosed. For example, tribromobismuthine mediated isomerization of a mixture of cis:trans tetrahydropyran II (48:50) in DCM afforded the trans-isomer of tetrahydropyran II in 87%.

IT 879544-22-6

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of trans-2,5-disubstituted tetrahydropyrans)

RN 879544-22-6 CAPLUS

CN Phenol, 4-[(2R,5R)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

IT 879544-24-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of trans-2,5-disubstituted tetrahydropyrans)

RN 879544-24-8 CAPLUS

CN Phenol, 4-(tetrahydro-5-propyl-2H-pyran-2-yl)- (CA INDEX NAME)

IT 700863-32-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of trans-2,5-disubstituted tetrahydropyrans)

RN 700863-32-7 CAPLUS

CN Phenol, 4-[(2R,5S)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

- L6 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2005:1169884 CAPLUS <<LOGINID::20080715>>
- DN 144:263983
- TI (2R\*,3R\*,6S\*)-N,6-Bis(4-fluorophenyl)-2-(4-hydroxyphenyl)-3,4,5,6-tetrahydro-2H-pyran-3-carboxamide
- AU Swamy, G. Y. S. K.; Ravikumar, K.; Wadhwa, L. K.; Saxena, Rahul; Singh, Saranjit
- CS Laboratory of X-ray Crystallography, Indian Institute of Chemical Technology, Hyderabad,  $500\ 007$ , India
- SO Acta Crystallographica, Section E: Structure Reports Online (2005), E61(11), o3608-o3610 CODEN: ACSEBH; ISSN: 1600-5368 URL: http://journals.iucr.org/e/issues/2005/11/00/bt6753/index.html
- PB Blackwell Publishing Ltd.
- DT Journal; (online computer file)
- LA English
- AB The mol. of the title compound, C24H21F2NO2, has a T-shaped form in the crystal structure. The central tetrahydropyran ring shows a chair conformation. All substituents are equatorially attached to this ring. The crystal packing is stabilized by N-H···O, O-H···O and C-H··· $\pi$ (arene) interactions. Crystallog. data are given.
- IT 876948-89-9P
  - RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of)
- RN 876948-89-9 CAPLUS
- CN 2H-Pyran-3-carboxamide, N,6-bis(4-fluorophenyl)tetrahydro-2-(4-hydroxyphenyl)-, (2R,3R,6S)-rel- (CA INDEX NAME)

Relative stereochemistry.

### RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2005:640097 CAPLUS <<LOGINID::20080715>>

DN 143:282602

TI Inhibitors of nitric oxide production from the rhizomes of Alpinia galanga: Structures of new 8-9' linked neolignans and sesquineolignan

AU Morikawa, Toshio; Ando, Shin; Matsuda, Hisashi; Kataoka, Shinya; Muraoka, Osamu; Yoshikawa, Masayuki

CS Kyoto Pharmaceutical University, Kyoto, 607-8412, Japan

SO Chemical & Pharmaceutical Bulletin (2005), 53(6), 625-630 CODEN: CPBTAL; ISSN: 0009-2363

PB Pharmaceutical Society of Japan

DT Journal

LA English

AB The 80% aqueous acetone extract from the rhizomes of Alpinia galanga showed nitric oxide (NO) production inhibitory activities in mouse peritoneal macrophages. From the aqueous acetone extract, three new 8-9' linked neolignans,

galanganal, galanganols A and B, and a sesquineolignan, galanganol C, were isolated together with nine known phenylpropanoids and p-hydroxybenzaldehyde. The structures of new neolignans were determined on the basis of physicochem. and chemical evidence. In addition, the inhibitory effects of the constituents from the rhizomes of A. galanga on NO production induced by lipopolysaccharide in mouse peritoneal macrophages were examined Among them, galanganal (IC50=68  $\mu$ M), galanganols B (88  $\mu$ M) and C (33  $\mu$ M), 1'S-1'-acetoxychavicol acetate (2.3  $\mu$ M), 1'S-1'-acetoxyeugenol acetate (11  $\mu$ M), trans-p-hydroxycinnamaldehyde (ca. 20  $\mu$ M), trans-p-coumaryl alc. (72  $\mu$ M), and trans-p-coumaryl diacetate (19  $\mu$ M) were found to show inhibitory activity.

IT 864073-18-7P, Galanganol C
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation) (novel neolignans and a sesquineolignan from the rhizomes of Alpinia galanga)

RN 864073-18-7 CAPLUS

CN 2H-Pyran-3-methanol, tetrahydro- $\alpha$ , 6-bis(4-hydroxyphenyl)-5-[(2E)-3-(4-hydroxyphenyl)-2-propen-1-yl]-, (3R,5R,6R)-rel- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.
Currently available stereo shown.

## RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2005:215581 CAPLUS <<LOGINID::20080715>>

DN 142:297993

TI Procedure for the hydrogenation of cyclohexene and dihydropyran derivatives

PA Merck Patent GmbH, Germany

SO Ger. Offen., 24 pp. CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
ΡI	DE 102004036068	A1	20050310	DE 2004-102004036068	20040724		
	CN 1626492	A	20050615	CN 2004-10057518	20040817		
	JP 2005060399	A	20050310	JP 2004-237823	20040818		
PRAI	DE 2003-10337836	IA	20030818				
OS	MARPAT 142:297993						

AB Cyclohexene and dihydropyran derivs. are hydrogenation using a transition metal complex of triphenylphosphine. Thus, 1-(2,3-difluoro-4-ethoxyphenyl)-4-(4-propylcyclohexyl)cyclohexene was reduced with Rh(PPh3)3Cl to give 76% trans-1-(2,3-difluoro-4-ethoxyphenyl)-4-(4-propylcyclohexyl)cyclohexane.

IT 847461-52-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (procedure for the hydrogenation of cyclohexene and dihydropyran derivs.)

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RN 847461-52-3 CAPLUS
CN 2H-Pyran, 2-(4-bromophenyl)-5-butyltetrahydro- (CA INDEX NAME)
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ANSWER 12 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
1.6
     2004:1059446 CAPLUS <<LOGINID::20080715>>
ΑN
     142:46069
DN
     Liquid-crystalline compounds having a tetrahydropyran ring
ΤI
     Kirsch, Peer; Poetsch, Eike; Manabe, Atsutaka
IN
PA
    Merck Patent G.m.b.H., Germany
SO
     PCT Int. Appl., 74 pp.
     CODEN: PIXXD2
DT
     Patent
LA
    German
FAN.CNT 1
                        KIND
                                          APPLICATION NO.
     PATENT NO.
                                DATE
                                                                  DATE
                              20041209
PΙ
     WO 2004106460
                         A1
                                           WO 2004-EP5539
                                                                   20040524
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
            LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
            NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
             SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
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20041216

20060719

20070329

DE 2004-102004025809

CN 2004-80016747

JP 2006-529903

US 2005-558209

20040524

20040524

20040524

20051125

US 20060289829 A1 20061228 US 7361388 B2 20080422 PRAI DE 2003-10324311 A 20030527 WO 2004-EP5539 W 20040524

Α1

Α

Τ

SN, TD, TG

DE 102004025809

JP 2007507439

MARPAT 142:46069

CN 1806028

OS GI

Ι

AB The invention relates to liquid-crystalline compds. of formula I (R11 = H, C1-15-alkyl, alkoxy, C2-15-alkenyl, alkenylxoy; X11 = F, C1, CN, NCS, SF5, C1-7-haloalkyl, haloalkoxy, haloalkenyl, haloakenylxoy; Z11-13 = -C2H4-, -C.tplbond.C-, -C2F4-, -CHO-, -OCH-, -COO-, -CF:CF-, -CH:CH, -CH:CF-, -CF2O-, -OCF2-, -(CH2)4-, -(CH2)3-, single bond; L11-16 = H, F), and to a method for the production thereof, their use in liquid-crystalline media, liquid-crystalline

media containing at least one above compound, and to electro-optical displays
 containing a liquid-crystalline medium of this type. There are one synthesis
 example

and one mixture example.

IT 700863-30-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(liquid crystal compound preparation; liquid-crystalline compds. having a tetrahydropyran ring for liquid crystal mixture suitable for liquid crystal display)

RN 700863-30-5 CAPLUS

CN 2H-Pyran, 2-(4-bromophenyl)tetrahydro-5-propyl-, (2R,5S)-rel- (CA INDEX NAME)

Relative stereochemistry.

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L6 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2004:1035071 CAPLUS <<LOGINID::20080715>>
- DN 142:30170
- TI Pyrans as liquid crystals for electrooptical and display devices
- IN Goulding, Mark John; Duffy, Warren; Adlem, Kevin; Kirsch, Peer; Hahn, Alexander; Poetsch, Eike; Binder, Werner; Meyer, Volker; Klasen-Memmer,

Melanie; Heckmeier, Michael; Luessem, Georg

PA Merck Patent GmbH, Germany

SO Eur. Pat. Appl., 22 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

FAN.CNI I																			
	PA:	FENT	NO.			KIND DATE		APE	APPLICATION NO.					DATE					
ΡI	EP	1482	021			A1	A1 20041201		EP	EP 2004-12212					20040524				
	EP	1482	021			В1		2007	0124										
		R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB, GF	:, II	Γ,	LI,	LU,	NL,	SE,	MC,	PT,	
			ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY, AI	, TF	۲,	BG,	CZ,	EE,	HU,	PL,	SK,	HR
	ΑT	3526	02			${f T}$		2007	0215	AT	2004	1 - 1	1221	2		2	0040	524	
	US	2005	0012	073		A1		2005	0120	US	2004	1 - 8	3547	73		2	0040	527	
	US	7022	865			В2		2006	0404										
PRAI	ΕP	2003	-119	06		A		2003	0527										
OS	MAI	RPAT	142:	3017	0														
GT																			

new

AB Tetrahydropyran derivs. comprising at least three cyclic rings and one aromatic end group of the formula I (X, Y = H, F, with the proviso that at least one of X and Y is F; Q = H, -CN, -NCS, -F, -Cl, -CF3, -OCF3, -OCHF2, -OCHFCF3, SF5 or -OCF2CF3); a process for preparing said tetrahydropyran derivs., and the use of said tetrahydropyran derivs. as a component in a liquid crystal composition The object of the present invention is to provide

tetrahydropyran derivs. which are suitable as components in liquid crystalline compns. and display devices, especially in nematic media having a balanced profile of the following properties: rotational viscosity, dielec. anisotropy and holding ratio; and having a good solubility for other components of liquid crystal compns. and a high pos. dielec. anisotropy.

IT 700863-30-5P 700863-32-7P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of liquid crystals for electrooptical and display devices)

RN 700863-30-5 CAPLUS

CN 2H-Pyran, 2-(4-bromophenyl)tetrahydro-5-propyl-, (2R,5S)-rel- (CA INDEX NAME)

Relative stereochemistry.

RN 700863-32-7 CAPLUS

CN Phenol, 4-[(2R,5S)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

# RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2004:962862 CAPLUS <<LOGINID::20080715>>

DN 141:403631

TI Liquid crystal compound and liquid crystal mixture showing improved physical properties for liquid crystal display

IN Kirsch, Peer; Hahn, Alexander; Poetsch, Eike; Meyer, Volker; Heckmeier, Michael; Klasen-Memmer, Melanie; Luessem, Georg; Hock, Christian

PA Merck Patent GmbH, Germany

SO Ger. Offen., 100 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

T. TJIA *	CIVI I				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	DE 10318420	A1	20041111	DE 2003-10318420	20030424
PRAI	DE 2003-10318420		20030424		
OS	MARPAT 141:403631				
GI					

$$R^{1}(A^{1}Z^{1})_{a}$$
  $(Z^{2}A^{2})_{b}$   $CF_{2}O(A^{3}Z^{3})_{c}$   $A^{4}R^{2}$ 

AB The title liquid crystal compound is represented by I (R1, R2 = H, halo, C1-15-alkyl, alkoxy; A1-4 = trans-1,4-cyclohexylene, 1,4-phenylene, etc.; Z1-3 = -COO-, -OCO-, -CF2O-, -OCF2-, etc.; a, b, c = 0-3). There are synthesis examples as well as 11 liquid crystal mixture examples.

IT 700863-30-5P 700863-32-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of liquid crystal compound and liquid crystal mixture showing improved

phys. properties for liquid crystal display)

RN 700863-30-5 CAPLUS

CN 2H-Pyran, 2-(4-bromophenyl)tetrahydro-5-propyl-, (2R,5S)-rel- (CA INDEX NAME)

Relative stereochemistry.

RN 700863-32-7 CAPLUS

CN Phenol, 4-[(2R,5S)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

- L6 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2004:466725 CAPLUS <<LOGINID::20080715>>
- DN 141:44938
- TI Liquid crystalline compound suitable for liquid crystal mixture of liquid crystal display
- IN Kirsch, Peer; Hahn, Alexander; Poetsch, Eike; Meyer, Volker; Heckmeier, Michael; Klasen-Memmer, Melanie; Luessem, Georg; Hock, Christian
- PA Merck Patent G.m.b.H., Germany
- SO Ger. Offen., 154 pp.

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CODEN: GWXXBX
DT
     Patent
LA
     German
FAN.CNT 1
     PATENT NO.
                       KIND
                               DATE
                                        APPLICATION NO.
                                                                  DATE
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                               _____
                                          ______
                                         DE 2003-10353658
WO 2003-EP12813
PΙ
     DE 10353658
                        A1
                               20040609
                                                                  20031117
     WO 2004048501
                        A1 20040610
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
             TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
             TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD,
     AU 2003302394
                         Α1
                             20040618 AU 2003-302394 20031117
     EP 1565540
                         Α1
                                20050824
                                           EP 2003-811758
                                                                  20031117
     EP 1565540
                         В1
                                20070926
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
                                         CN 2003-80104414 20031117
                               20060104
     CN 1717468
                        Α
                                          JP 2004-554363
     JP 2006508150
                         Τ
                               20060309
                                                                  20031117
     AT 374232
                         Τ
                               20071015
                                           AT 2003-811758
                                                                  20031117
                        A1 20060323
     US 20060061699
                                           US 2005-536808
                                                                  20050527
     US 7291367
                        В2
                             20071106
PRAI DE 2002-10255311
                        A1 20021127
                        W
     WO 2003-EP12813
                               20031117
    MARPAT 141:44938
OS
GΙ
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$$R^{1}$$
 - (A<sup>1</sup>-Z<sup>1</sup>)a - (Z<sup>2</sup>-A<sup>2</sup>)b-CF<sub>2</sub>O-(A<sup>3</sup>-Z<sup>3</sup>)c-A<sup>4</sup>-R<sup>2</sup>

AB The title liquid crystalline compound is represented by a general formula I (R1, R2

= H, halo, C1-15-alkyl, alkoxy; A1-4 = 1,4-trans-cyclohexylene,

1,4-phenylene, etc.;Z1-3 = -COO-, -OCO-, -CF2O-, etc.; a, b, c = 0-3; a + b + c  $\leq 3$ ). Synthesis examples and 45 mixture examples are given.

IT 700863-30-5P 700863-32-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of liquid crystalline compound suitable for liquid crystal mixture of liquid  $% \left( 1\right) =\left( 1\right) +\left( 1\right) +$ 

crystal display)

RN 700863-30-5 CAPLUS

CN 2H-Pyran, 2-(4-bromophenyl)tetrahydro-5-propyl-, (2R,5S)-rel- (CA INDEX NAME)

Relative stereochemistry.

RN 700863-32-7 CAPLUS

CN Phenol, 4-[(2R,5S)-tetrahydro-5-propyl-2H-pyran-2-yl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

- L6 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2004:466724 CAPLUS <<LOGINID::20080715>>
- DN 141:23420
- TI Preparation of tetrahydropyran derivatives
- IN Kirsch, Peer; Hahn, Alexander; Poetsch, Eike; Binder, Werner; Meyer, Volker
- PA Merck Patent G.m.b.H., Germany
- SO Ger. Offen., 31 pp.

CODEN: GWXXBX

- DT Patent
- LA German
- FAN.CNT 1

	PATEN	r no.			KIN	D	DATE			APPL	ICAT	ION 1	NO.		D.	ATE	
						_									_		
ΡI	DE 10	353656			A1		2004	0609		DE 2	003-	1035	3656		2	0031	117
	WO 20	040483	57		A1		2004	0610	,	WO 2	003-	EP12	812		2	0031	117
	W	: AE,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FΙ,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	KΖ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MΖ,	ΝI,	NO,	NΖ,	OM,
		PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	ΤJ,	TM,	TN,
		TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW			

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RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
             TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     AU 2003288078
                          Α1
                                 20040618
                                            AU 2003-288078
                                                                    20031117
     EP 1565450
                          Α1
                                20050824
                                            EP 2003-779946
                                                                    20031117
     EP 1565450
                          В1
                                 20070704
           AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
         R:
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     CN 1717400
                                20060104
                                            CN 2003-80104460
                          Α
                                                                    20031117
     JP 2006515283
                          Τ
                                 20060525
                                             JP 2004-554362
                                                                    20031117
     AT 366247
                          Τ
                                20070715
                                            AT 2003-779946
                                                                    20031117
     US 20060058527
                          A1
                                20060316
                                            US 2005-536803
                                                                    20050527
PRAI DE 2002-10255312
                                20021127
                          Α1
     WO 2003-EP12812
                                 20031117
                          W
OS
     CASREACT 141:23420; MARPAT 141:23420
GΙ
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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The invention concerns tetrahydropyran derivs. I [R11 = H, F, Cl, Br, I, CN, aryl, heterocyclyl, C1-15-alkyl {optionally containing internal, C.tplbond.C, CH:CH, O, C(:0), C(:0)0, O-C(:0)}, C1-15-haloalkyl;  $A = \frac{1}{2}$ cyclohexane-1,4-diyl, tetrahydropyran-2,5-diyl, pyrimidine-2,5-diyl; m = 0 - 2; Z11 = CH2CH2, CF2CF2, CF2CH2, CH2CF2, CH2O, OCH2, CF2O, OCF2; ₩ = CH, C:; B, D = cyclohexane-1, 4-diyl, B', D'; n = 0, 1; Y11 = :0, C(SR12)(SR13), :CF2, H, F, Cl, Br, I, CN, OH, SH, COR14, OSO2R15, C(:S+R12)(SR13)X'-, B(OR16)(OR17), BF3-M+, Si(OR18)(OR19)(OR20), C1-15-alkyl, C1-15-haloalkyl; Y12, Y13 = H, C1-15-haloalkyl, C1-15-alkyl; L1, L2, L3 = H, F; R12, R13 = (un) branched C1-15-alkyl; R12R13 = (CH2)p; p = 2 - 6; R14 = OH, O-aryl, O-aralkyl, O-alkyl, Cl, Br, aryl, aralkyl, alkyl; R15 = aryl, aralkyl, C1-15-alkyl, C1-15-haloalkyl; R16, R17 =C1-15-alkyl, C1-15-haloalkyl; R16R17 = (CH2)p; R18, R19, R20 =(un)branched C1-15-alkyl; M+ = alkali metal cation, NH4+; X' = weak coordination anion; etc.] and procedure for their production One procedure for the the preparation of I is characterized by: (i) reaction of R11AmZ11CH2CHO with Y12CH:C(Y13)CO2R31 (R31 = C1-15-alkyl); (ii) cyclization of R11AmZ11CH(CHO)CHY12CHY13CO2R31; (iii) condensation of pyrone II (X = 0) with CF2Br2 in the presence of P[N(R21)2]3, P[N(R21)2]2(OR22), or P[N(R21)2](OR22)2 (R21, R22 = C1-15-alkyl) to give pyran II (X = CF2) or condensation with CHG(SR12)(S13) [G = P(OCH2R23)3; R23 = C1-15-perfluoroalkyl, SiMe3, SiEt3] to give pyran II [X = C(SR12)(SR13)]. Thus, pyran III was prepared from Me(CH2)7CHO, via cyclocondensation with H2C:CHCO2Me to give 5-heptyl-2-pyranone, reaction with 4-BrC6H4Li followed by Et3SiH and BF3OEt2 to give 2-(4-bromophenyl)-5-heptylpyran, reaction with B(OMe)3 followed by acid hydrolysis to give [4-(5-heptylpyran-2-yl)phenyl]boronic acid, basic hydrolysis to give 2-(4-Hydroxyphenyl)-5-heptylpyran, hydrogenation to give 2-(4-oxocyclohexyl)-5-heptylpyran, condensation of with 2-(trimethylsilyl)-1,3-dithiane to give the cyclohexylidenedithiane, and addition reaction of 3,4,5-trifluorophenol followed by fluorination with Et3N·3HF.

IT 700819-43-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrogenation of; preparation of tetrahydropyran derivs.)

700819-43-8 CAPLUS RN

CN Phenol, 4-(5-heptyltetrahydro-2H-pyran-2-yl)- (CA INDEX NAME)

700819-33-6P ΤТ

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with tri-Me borate; preparation of tetrahydropyran

derivs.)

RN 700819-33-6 CAPLUS

CN 2H-Pyran, 2-(4-bromophenyl)-5-heptyltetrahydro- (CA INDEX NAME)

- L6 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
- 2003:75149 CAPLUS <<LOGINID::20080715>> ΑN

DN 138:278701

r-2, c-6-Bis (4-chlorophenyl)-3,5-dimethyltetrahydropyran-t-4-ol TI

- Krishnamoorthy, Belli Sundaram; Sarangarajan, Thanjavur Ramabhadran; ΑU Thanikasalam, Kanagasabapathy; Panchanatheswaran, Krishnaswamy; Jeyaraman, Ramasubbu
- CS Department of Chemistry, Bharathidasan University, Tiruchirappalli, 620 024, India
- Acta Crystallographica, Section E: Structure Reports Online (2003), SO E59(2), o111-o113 CODEN: ACSEBH; ISSN: 1600-5368

URL: http://journals.iucr.org/e/issues/2003/02/00/ob6197/index.html International Union of Crystallography

- PΒ
- DT Journal; (online computer file)

English LA

AΒ Crystals of the title compound are monoclinic, space group P21/c, with a 12.1315(9), b 11.7075(10), c 26.177(3) Å,  $\beta$  99.728(9)°; Z = 4 (2 mols./Z), dc = 1.273; R = 0.053, Rw(F2) = 0.146 for 6670reflections. The structure reveals a chair conformation for the pyran ring in which the hydroxyl group is axially oriented. All the other substituents occupy equatorial positions.

ΙT 503598-15-0 RL: PRP (Properties) (crystal structure of)

RN 503598-15-0 CAPLUS

CN 2H-Pyran-4-ol, 2,6-bis(4-chlorophenyl)tetrahydro-3,5-dimethyl-,  $(2\alpha,3\beta,4\beta,5\beta,6\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

# RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 18 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1985:406353 CAPLUS <<LOGINID::20080715>>

DN 103:6353

OREF 103:1147a,1150a

TI 1,4-Dioxanes

IN Eidenschink, Rudolf; Weber, Georg

PA Merck Patent G.m.b.H., Fed. Rep. Ger.

SO Ger. Offen., 40 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

FAN.CNI I				
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE 3322982	A1	19850103	DE 1983-3322982	19830625
GB 2142020	A	19850109	GB 1984-15518	19840618
JP 60023378	A	19850205	JP 1984-127671	19840622
US 4755323	A	19880705	US 1986-839293	19860313
PRAI DE 1983-3322982	A	19830625		
US 1984-624172	A1	19840625		
OS MARPAT 103:6353				
GI				

AB Dioxanes I [R1 = C1-10 alkyl (optionally with 1 or 2 CH2 replaced by 0), F, C1, Br, cyano; R2 = R1, H; Z1, Z2 = C(0)0, OC(0), CH2CH2, OCH2, CH2O, bond; Z3, Z4 = 1,4-C6H4, 1,4-cyclohexylene, 1,3-dioxane-2,5-diyl, 1,4-dioxane-2,5-diyl, 1,4-piperidinediyl, 1,4-bicyclo[2.2.2]octylene, 2,5-pyrimidinediyl (un)substituted by 1-4 F atoms; m, n = 0-3; m + n = 1-3], useful as components of liquid crystalline dielecs., were prepared Treating

PhCOMe at 2° with SnCl4 at <20°, then with 4-methylstyrene oxide 1 h at 20° gave trans-II.

IT 96787-16-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as liquid crystalline dielec.)

RN 96787-16-5 CAPLUS

CN Benzonitrile, 4-(tetrahydro-5-pentyl-2H-pyran-2-yl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L6 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1985:195308 CAPLUS <<LOGINID::20080715>>

DN 102:195308

OREF 102:30493a,30496a

TI Tetrahydropyrans for liquid crystal display devices

IN Eidenschink, Rudolf; Krause, Joachim; Fuss, Peter

PA Merck Patent G.m.b.H., Fed. Rep. Ger.

SO Ger. Offen., 60 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

ΡI	DE 3306960	A1	19840830	DE 1983-3306960	19830228
	EP 117476	A1	19840905	EP 1984-101456	19840213
	EP 117476	В1	19870916		
	R: CH, DE, FR,	GB, LI			
	JP 59164788	A	19840917	JP 1984-35455	19840228
	US 4818431	A	19890404	US 1986-933953	19861124
PRAI	DE 1983-3306960	A	19830228		
	US 1984-583507	A1	19840224		
OS	MARPAT 102:195308				
GI					

$$R(Z)_{m}Z^{2} \longrightarrow Z^{3}(Z^{1})_{n}R^{1}$$

$$R(Z)_{m}Z^{2} \longrightarrow Z^{3}(Z^{1})_{n}R^{1}$$

$$II$$

Tetrahydropyran derivs. of the formulas I and II (R = C1-10 alkyl or alkyl in which 1 or 2 CH2 groups are replaced with 0, F, Cl, Br, or CN; R1 = H or R; Z, Z1 = unsubstituted or 1-4 substituted 1,4-phenylene, 1,4-cyclohexylene, 1,3-dioxan-2,5-diyl, piperindin-1,4-diyl, 1,4-bicyclo[2.2.2]octylene, or pyrimidin-2,5-diyl; Z2, Z3 = CO2, O2C, CH2CH2, OCH2, CH2O, or a bond; m, n = 0, 1, 2, or 3; and m + n =  $\geq$ 1 or  $\leq$ 3) as well as their acid addition salts are described for use in liquid crystal compns. for display devices. These compds. can be used to produce stable liquid crystal phases with a strongly neg as well as pos. dielec. anisotropy, a small threshold potential electrooptical effect, a highly variable optical anisotropy, and a comparably low viscosity. Thus, a typical liquid crystal composition with a neg. dielec. anisotropy consisted

of 2-p-elhoxyphenyl-5-propyltetrahydropyran 25, trans-1-p-butoxyphenyl-4-propylcyclohexane 25, p-pentylphenyl trans-4-pentylcyclohexanecarboxylate 15, p-ethoxyphenyl trans-4-propylcyclohexanecarboxylate 15, 4-(trans-4-petnylcyclohexyl)-4'-(trans-4- propylcyclohexyl)biphenyl 10, and 4-butyl-2-cyanophenyl p-trans-4-propylcyclohexylbenzoate 10% showed a clearing point of 61°.

IT 95377-05-2 95377-06-3

RL: TEM (Technical or engineered material use); USES (Uses) (liquid crystal compns. containing, for electrooptical display devices) 95377-05-2 CAPLUS

CN Benzonitrile, 4-(tetrahydro-5-propyl-2H-pyran-2-yl)- (CA INDEX NAME)

RN

RN 95377-06-3 CAPLUS

CN Benzonitrile, 4-(5-butyltetrahydro-2H-pyran-2-yl)- (CA INDEX NAME)

IT 95377-14-3P 95391-61-0P 95391-62-1P

95391-63-2P

RL: PREP (Preparation)

(preparation and liquid crystal display applications of)

RN 95377-14-3 CAPLUS

CN Benzonitrile, 4-(tetrahydro-5-pentyl-2H-pyran-2-yl)- (CA INDEX NAME)

RN 95391-61-0 CAPLUS

CN 2H-Pyran, 2-(4-chlorophenyl)tetrahydro-5-pentyl- (CA INDEX NAME)

RN 95391-62-1 CAPLUS

CN 2H-Pyran, 2-(4-bromophenyl)tetrahydro-5-pentyl- (CA INDEX NAME)

RN 95391-63-2 CAPLUS

CN 2H-Pyran, 2-(4-fluorophenyl)tetrahydro-5-pentyl- (CA INDEX NAME)

ΙT 95377-38-1

> RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with hexyl iodide)

RN 95377-38-1 CAPLUS

Phenol, 4-(tetrahydro-5-pentyl-2H-pyran-2-yl)- (CA INDEX NAME) CN

L6 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

ΑN

99:37717 DN

OREF 99:5921a,5924a

Base strengths of 4-aminooxanes (tetrahydropyrans), (methylamino)oxanes, ΤI (dimethylamino)oxanes, (methylamino)thianes, and (dimethylamino)thianes

ΑU Chandrasekara, Nallappan; Subramanian, Pullachipatti K.; Ramalingam, Kondareddiar; Satyamurthy, Nagichettiar; Berlin, K. Darrell

Dep. Chem., PSG Coll. Arts and Sci., Coimbatore, 641 014, India CS SO

Journal of Organic Chemistry (1983), 48(10), 1597-601 CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

English LA

GΙ

AΒ The pKa values of numerous title compds. were interpreted in terms of steric effects, and conformations were suggested. For example, a twist conformation was suggested for I. The twist form avoids severe nonbonded interactions. 1H NMR data supported a nonchain form for several of the compds. Solvation effects were discussed.

85336-33-0P 85336-39-6P ΙT

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 85336-33-0 CAPLUS

CN 2H-Pyran-4-amine, 2,6-bis(4-chlorophenyl)tetrahydro-3,5-dimethyl-,  $(2\alpha,3\beta,4\beta,5\beta,6\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN

RN 85336-39-6 CAPLUS

CN 2H-Pyran-4-amine, 2,6-bis(4-chlorophenyl)tetrahydro-3,5-dimethyl-,  $(2\alpha, 3\beta, 4\alpha, 5\beta, 6\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

L6 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1979:86324 CAPLUS <<LOGINID::20080715>>

DN 90:86324

OREF 90:13665a,13668a

TI Kinetics of acetylation of some epimeric tetrahydropyran-4-ols

AU Baliah, V.; Mangalam, G.

CS Dep. Chem., Annamalai Univ., Annamalainagar, India

SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1978), 16B(9), 827-8 CODEN: IJSBDB; ISSN: 0376-4699

DT Journal

LA English

GΙ

AB Second-order rate consts. were determined for the acetylation of I (R, R1 = H, Me, Et; R2 = H, 4-Cl, 4-MeO, 3-NO2, 4-Me) having the OH group equatorial ( $\alpha$ ) or axial ( $\beta$ ). The  $\alpha$  epimer reacted faster than the  $\beta$ . A 3-Et group accelerated the acetylation of the  $\alpha$  epimer and inhibited that of the  $\beta$  epimer. When R = R1 = Me, the rate was lowered for both epimers.

IT 67405-38-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(acetylation of, kinetics of)

RN 67405-38-3 CAPLUS

CN 2H-Pyran-4-ol, 2,6-bis(4-chlorophenyl)tetrahydro-3,5-dimethyl- (9CI) (CA INDEX NAME)

L6 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1978:508937 CAPLUS <<LOGINID::20080715>>

DN 89:108937

OREF 89:16765a,16768a

TI Preparation and stereochemistry of some substituted tetrahydropyran-4-ones and tetrahydropyran-4-ols

AU Baliah, V.; Mangalam, G.

CS Dep. Chem., Annamalai Univ., Annamalainagar, India

SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1978), 16B(3), 213-15 CODEN: IJSBDB; ISSN: 0376-4699

DT Journal

LA English

OS CASREACT 89:108937

AB 3-Ethyl-2,6-diphenyltetrahydropyran-4-one and 2,6-diaryl-3,5-dimethyltetrahydropyran-4-ones (aryl = p-RC6H4; R = Cl, MeO, Me; m-O2NC6H4) were prepared A probable conformation is suggested for 3-methyl-2,6-diphenyltetrahydropyran-4-one on the basis of NMR spectrum. The reduction of tetrahydropyran-4-ones by different methods afforded epimeric pairs of tetrahydropyran-4-ols which were separated by column chromatog. The conformations of the epimeric alcs. are discussed.

IT 67405-38-3P

RN 67405-38-3 CAPLUS

CN 2H-Pyran-4-ol, 2,6-bis(4-chlorophenyl)tetrahydro-3,5-dimethyl- (9CI) (CA INDEX NAME)